N-Cycloheptyl-N'-phenylurea 19095-79-5 | DTXSID10172606

Model Performance

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Model	I)ata
Widdei	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 3.57e-03 mol/L

Global applicability domain: Inside

Local applicability domain index: 5.60e-01

Confidence level: 4.41e-01

Nearest Neighbors from the Training Set

Image not found

Norea

Measured: 6.75e-04 Predicted: 1.66e-03

Image not found

Siduron

Measured: 7.75e-05 Predicted: 2.20e-03

Image not found

Meperidine

Measured: 1.30e-02 Predicted: 1.38e-02

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4-Dimethylaminoantipyrine

Measured: 2.35e-01 Predicted: 4.06e-01